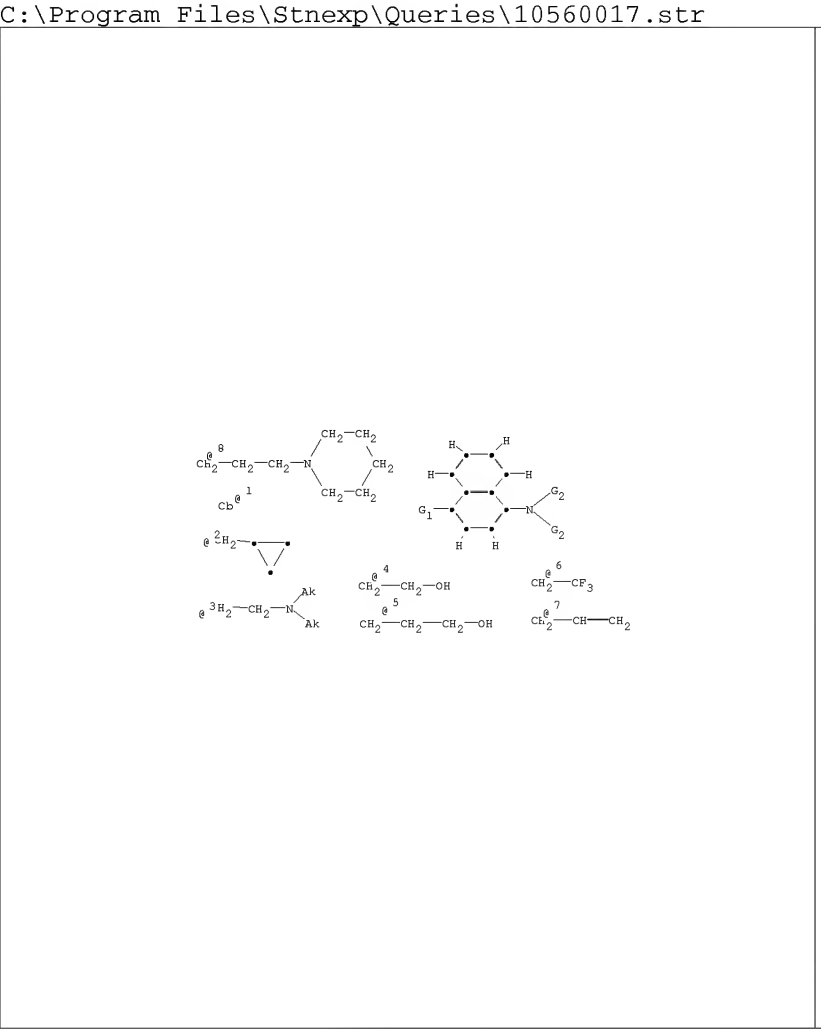
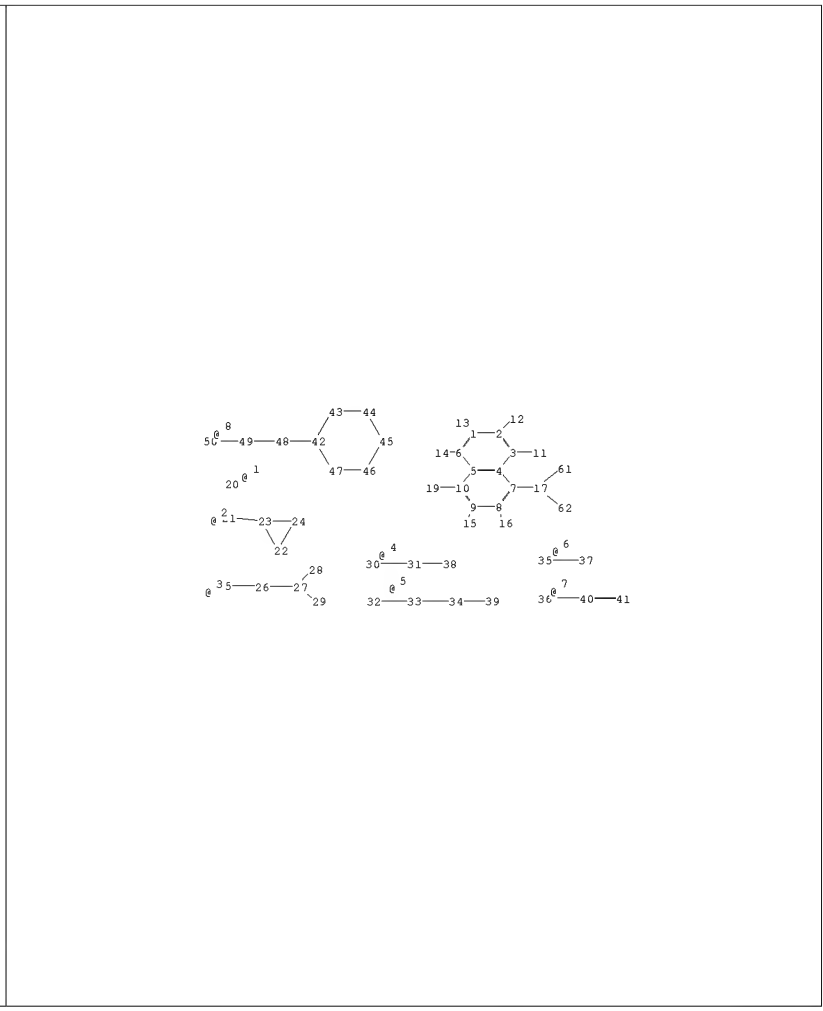
C:\Program Files\Stnexp\Queries\10560017.str





chain nodes :
11 12 13 14 15 16 17 19 20 21 25 26 27 28 29 30 31 32 33 34 35 36 37 38
39 40 41 48 49 50 61 62
ring nodes :
1 2 3 4 5 6 7 8 9 10 22 23 24 42 43 44 45 46 47
chain bonds :
1-13 2-12 3-11 6-14 7-17 8-16 9-15 10-19 17-61 17-62 21-23 25-26 26-27 27-28
27-29 30-31 31-38 32-33 33-34 34-39 35-37 36-40 40-41 42-48 48-49 49-50
ring bonds :
1-2 1-6 2-3 3-4 4-5 4-7 5-6 5-10 7-8 8-9 9-10 22-23 22-24 23-24 42-43 42-47
43-44 44-45 45-46 46-47
exact/norm bonds :
7-17 10-19 17-61 17-62 22-23 22-24 23-24 27-28 27-29
exact bonds :
1-13 2-12 3-11 6-14 8-16 9-15 21-23 25-26 26-27 30-31 31-38 32-33 33-34 34-39
35-37 36-40 40-41 42-43 42-47 42-48 43-44 44-45 45-46 46-47 48-49 49-50
normalized bonds :
1-2 1-6 2-3 3-4 4-5 4-7 5-6 5-10 7-8 8-9 9-10
isolated ring systems :
containing 42 :

G1:CN,NO2,X

G2:H,CH3,Et,n-Pr,i-Pr,n-Bu,i-Bu,s-Bu,t-Bu,[*1],[*2],[*3],[*4],[*5],[*6],[*7],[*8]

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:CLASS
12:CLASS 13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:CLASS 19:CLASS 20:Atom 21:CLASS
22:Atom 23:Atom 24:Atom 25:CLASS 26:CLASS 27:CLASS 28:CLASS 29:CLASS 30:CLASS 31:CLASS
32:CLASS 33:CLASS 34:CLASS 35:CLASS 36:CLASS 37:CLASS 38:CLASS 39:CLASS 40:CLASS
41:CLASS 42:Atom 43:Atom 44:Atom 45:Atom 46:Atom 47:Atom 48:CLASS 49:CLASS 50:CLASS
61:CLASS 62:CLASS
Generic attributes :
20:

Saturation : Saturated
Number of Carbon Atoms : less than 7
Type of Ring System : Monocyclic